

ABSTRACT OF THE DISCLOSURE

The invention provides a method for identifying a pharmacocluster. The method includes the steps of (a) determining bound conformations of a ligand bound to
5 different polypeptides, and (b) clustering two or more bound conformations of the ligand having substantially the same bound conformation, thereby identifying a pharmacocluster. The invention also provides a method for identifying a member of a pharmacocluster. The invention also provides a
10 method for identifying a polypeptide pharmacofamily. The method includes the steps of (a) determining bound conformations of a ligand bound to different polypeptides of a polypeptide family, and (b) identifying two or more bound conformations of the ligand having substantially different
15 bound conformations, thereby identifying at least two polypeptide pharmacofamilies exhibiting binding specificity for the two or more substantially different bound conformations of the ligand.